

# Combustion Research Facility NEWS



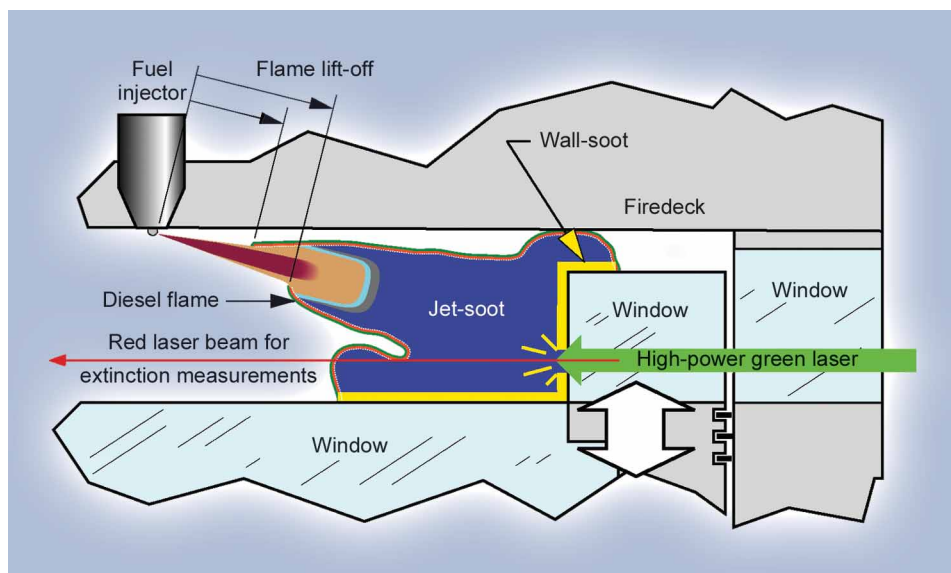
## Influence of Air Entrainment and Fuel Chemistry on Soot Formation Studied in a Heavy-Duty Diesel Engine

**D**iesel engine manufacturers continue to be concerned about meeting ever-tightening standards for particulate matter emissions. In efforts to find ways to reduce pollutant emissions from diesel engines, Sandia scientists are using optical diagnostics to understand the processes that affect the formation and ultimate emission of these pollutants.

In a diesel engine, the combusting fuel jet is essentially a lifted flame. Recent research at the CRF has shown that the lift-off length of a steady diesel flame, through its influence on air entrainment and mixing prior to reaction, can significantly affect soot formation, which is a major component of diesel particulate matter emissions (CRF News, July/August 2001). In addition, the molecular structure of the fuel molecules, including the fraction of aromatic hydrocarbons and/or oxygenated fuel molecules, can affect in-cylinder soot formation.

In work supported by DOE's Office of Heavy Vehicle Technologies, Mark Musculus has been using laser and imaging diagnostics to measure the combined effects of air entrainment and fuel molecular structure on in-cylinder soot formation in an optically accessible heavy-duty diesel engine. A variety of fuels were examined, ranging from conventional diesel fuels to a Fischer-Tropsch-like paraffinic fuel that was blended with various quantities of a low-sooting oxygenated fuel.

The quantity of soot within the reacting diesel jet, or "jet-soot," (shown in blue in Figure 1) was measured using a continuous-wave laser-based light extinction diagnostic. A second high-power, pulsed laser (shown in green) was employed to blast soot deposits (shown in yellow) from the window surfaces to facilitate direct measurement of jet-soot through the laser-cleaned windows. As shown in Figure 2, the formation of jet-soot (green



**Figure 1.** To better understand the effects of air entrainment and fuel molecular structure on in-cylinder soot formation in diesel engines, Mark Musculus has been using a continuous-wave laser-based light extinction diagnostic to measure the amount of jet-soot deposited on the windows of an optically accessible diesel engine. Above is a partial cross-sectional view of the optically accessible diesel engine combustion chamber.

squares) decreased nearly linearly with the oxygen-to-carbon ratio of the oxygenated fuel blends.

With more highly sooting fuels, the jet-soot cloud becomes optically opaque, and it cannot be directly probed using this extinction diagnostic. To extend the measurement range to include highly sooting fuels, the pulsed high-power window-cleaning laser was turned off, and the rate of deposition of soot on the surface of a window mounted to the piston was measured after each fired cycle using the laser extinction technique (see Figure 1). As shown in Figure 2, the jet-soot (green squares) and wall-soot (green circles) measurements for oxygenated fuels were in agreement. Then, using the wall-soot diagnostic to indirectly measure soot formation for more highly sooting fuels, extinction measurements showed that

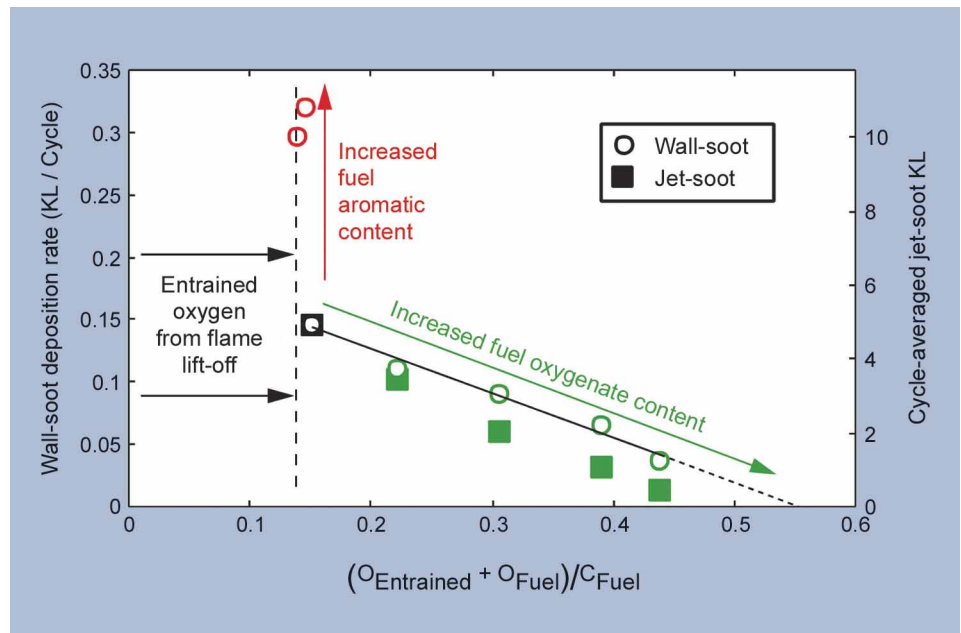
conventional diesel fuels (shown in red in Figure 2), which contain 25–30% aromatic molecules, had nearly twice the in-cylinder soot of a comparable paraffinic hydrocarbon fuel (shown in black in Figure 2).

Finally, to assess the affects of air entrainment on soot formation, imaging of the naturally occurring ultraviolet light emission from the hot flame (OH chemiluminescence) was employed to measure the lift-off length of the diesel flame. Using spray entrainment correlations, the lift-off length can provide an estimate of the air entrainment upstream of the flame lift-off length. Under the conditions tested, the lift-off lengths of the fuels in this study were all very similar, and the resulting air entrainment rates were also very similar between fuels. Thus, the effects of air entrainment essentially resulted in a

uniform rightward shift of the extinction data for all fuels, as shown in Figure 2.

These measurements provide new insight into the relative importance of the roles that fuel-air mixing and fuel-bound oxygen play in reducing soot emissions from diesel engines.

**Figure 2.** Measurements of soot through the laser-cleaned windows of a diesel engine revealed that the formation of jet-soot (green squares) decreased nearly linearly with the oxygen-to-carbon ratio of the oxygenated fuel blends. (KL=optical density of the soot in the path of the laser beam.) When more highly sooting fuels were indirectly measured using the wall-soot diagnostic, it was found that conventional diesel fuels (shown in red) had nearly twice the in-cylinder soot of a comparable paraffinic hydrocarbon fuel (shown in black).



## The CRF Hosts the Advanced Research Planning Workshop



The Advanced Research Planning Workshop for DOE/Office of Fossil Energy's (FE) Advanced Research Program took place on June 12 and 13, 2002 at the CRF. Approximately 40 attendees from private industry, universities, national laboratories, and federal agencies visited the CRF for the two-day workshop. Marvin Singer, Director of the Office of Advanced Research (AR), opened the meeting and summarized the need to obtain stakeholder input on research needs and current opportunities for the FE Program. Bob Romanosky, AR Product Manager from the National Energy Technology Laboratory (NETL), outlined the current activities in the Program. David Bader and Bill Kirchoff from DOE's Office of Science, described two new thrusts in "Scientific Discovery through Advanced Computing and Nanoscience." Professor Adel Sarofim from the University of Utah, provided a glimpse of recently successful efforts to extend research results into practice through computer simulations. The remainder of the workshop was devoted to defining the barriers to achieving the goals of the program and ways to overcome those barriers. Don Hardesty closed the workshop with a tour of the CRF.



# Awards

## Siebers and Miles Win SAE Honors

Dennis Siebers and Brian Higgins have been given the 2001 Harry L. Horning Memorial Award by The Society of Automotive Engineers (SAE) for their paper "Flame Lift-Off on Direct-Injection Diesel Sprays Under Quiescent Conditions." The Horning Award is one of the highest honors that can be given for automotive research. Thomas Ryan, Vice Chairman of the 2001 Horning Memorial Board of Awards, presented the award during The Diesel Emission Control Technologies Session on Thursday, October 24, 2002. Dennis joined Sandia in 1976 and is a Distinguished Member of the Technical Staff. He recently became Manager of the Engine Combustion Department at the CRF. Brian, currently an Assistant Professor at the California Polytechnic State University in San Luis Obispo, California, worked with Dennis in the Combustion Engines Department at the CRF as a post-doctoral research fellow between 1997 and 2000.



Dennis Siebers, 2001 winner of the Horning Award



Paul Miles, recipient of the SAE's McFarland Award, shown working on the high-speed direct-injection diesel engine

The Society of Automotive Engineers recognized Paul Miles' outstanding contributions toward the work of the SAE Engineering Meetings Board by presenting him with the Forest R. McFarland Award at the SAE Honors Convocation. This award annually recognizes automotive engineers who make exceptional contributions through development and dissemination of technical information and who facilitate or enhance interchanges of technical information.

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## CRF Scientists Present Papers in Japan

The CRF was well represented at the 29th International Symposium on Combustion in Sapporo, Japan. Sandians chairing symposium sessions included Jay Keller—Internal Combustion Engines, Steve Margolis—Laminar Flames, Jackie Chen—Laminar Flames, Don Hardesty—Stationary Combustion, and Rob Barlow—Turbulent Combustion. Alan Kerstein delivered a topical review entitled “Turbulence in Combustion: Modelling Challenges.” Papers coauthored by CRF staff members (names in plain text) are listed below.

***Simultaneous Laser Raman-Rayleigh LIF Measurements and Numerical Modeling Results of a Lifted Turbulent  $H_2/N_2$  Jet Flame in a Vitiated Coflow***, Cabra, R., Myhrvold, T., Chen, J.Y., and Dibble, R.W. (UC Berkeley) and Karpetis, A.N. and Barlow, R.S.

***A Theoretical Analysis of the  $CH_3 + H$  Reaction: Isotope Effects, the High Pressure Limit, and Transition State Recrossing***, Klippenstein, S.J., Georgievski, Y., and Harding, L.B. (Argonne National Lab)

***Measurement of Laminar Flame Speeds Through Digital Particle Image Velocimetry: Mixtures of Methane and Ethane with Hydrogen, Oxygen, Nitrogen, and Helium***, Dong, Y. (USC), Vagelopoulos, C.M., and Egolfopoulos, G.N. and Spedding, G.R. (USC)

***Combustion of Hydrogen Enriched Methane in a Lean Premixed Swirl-Stabilized Burner***, Schefer, R.W., Wicksall, D.M., and Agrawal, A.K. (University of Oklahoma)

***High-Pressure Single-Pulse Shock Tube Investigation of Rich and Stoichiometric Ethane Oxidation***, Tranter, R.S., Ramamoorthy, H., Raman, A., and Brezinsky, K. (University of Illinois) and Allendorf, M.D.

***Measurements and Modeling of Reynolds Stress and Turbulence Production in a Swirl-Supported, Direct-Injection Diesel Engine***, Miles, P.C., Megerle, M., Nagel, Z., and Reitz, R. (University of Wisconsin) and Sick, V. (University of Michigan)

***An Investigation of Diesel Soot Formation Processes Using Micro-Orifices***, Pickett, L.M. and Siebers, D.L.

***Intrusive-Limit Deflagrations in Confined Porous Energetic Materials***, Margolis, S.B., Telengator, A.M., and Williams, F.A. (UC San Diego)

***An LIF Equivalence Ratio Imaging Technique for Multi-component Fuels in an IC Engine***, Han, D. and Steeper, R.R.

***Role of Transport Properties in the Transient Response of Premixed Methane-Air Flame***, Najm, H.N., Knio, O.M. (Johns Hopkins), and Paul, P.H. (Eksigent)

***Effects of Unsteady Scalar Dissipation Rate on Ignition in Counterflow***, Mason, S.D., Chen, J.H., and Im, H.G. (University of Michigan)

***Effects of Flow and Chemistry on OH Levels in Premixed Flame-Vortex Interactions***, Vagelopoulos, C.M. and Frank, J.H.

***High-Temperature Combustion in Autoigniting Non-Homogeneous Hydrogen-Air Mixtures***, Echekki, T. (North Carolina State University) and Chen, J.H.

***Reaction Rate, Mixture Fraction, and Temperature Imaging in Turbulent Methane/Air Jet Flames***, Frank, J.H., Kaiser, S.A., and Long, M.B. (Yale)

***Structure of Turbulent Non-Premixed Jet Flames in a Diluted Hot Coflow***, Dally, B.B. (University of Adelaide) and Karpetis, A.N.

***Swirling Turbulent Non-Premixed Flames of Methane: Flowfield and Compositional Structure***, Kalt, P.A.M., Al-Abdeli, Y.M., and Masri, A.R. (University of Sydney) and Barlow, R.S.

***REMPI Temperature Measurement in Molecular Beam Sampled Low-Pressure Flames***, Kamphus, M., Liu, N.-N., and Atakan, B. (University of Bielefeld), and McIlroy, A. and Qi, F.

***Measurements of Scalar Dissipation in a Turbulent Piloted Methane/Air Jet Flame***, Karpetis, A.N. and Barlow, R.S.

***Measurements of NO Distributions and Fluorescence Lifetimes in a Non-Premixed Counterflow  $CH_4$ /Air Flame Using Picosecond Time-Resolved Laser-Induced Fluorescence***, Driscoll, J.J., Sick, V. (University of Michigan), and Schrader, P.E. and Farrow, R.L.

***The Existence of Young Soot in the Exhaust of Inverse Diffusion Flames***, Blevins, Linda., Fletcher, R.A., Benner Jr. G.A., Steel, E.B., and Mulholland, G.W. (NIST)

## Uncertainty Quantification in Flow Simulations of Natural Convection in a Heated Cavity

Knowing how uncertainty affects a final result can be the key to optimizing an engineering system or validating a computational model. The goal of uncertainty quantification (UQ) research is to learn how uncertainty in physical parameters propagates through computational models. Habib Najm, Matthew Reagan, and Bert Debuschere of the CRF, along with Roger Ghanem and Omar Knio at Johns Hopkins University and Olivier Le Maître of the Université d'Evry Val d'Essonne, have been developing the tools and applications needed to implement UQ in a wide range of applications. Studying natural convection in a heated cavity, they have demonstrated that the ability to proceed from a stochastic representation of inputs to a probabilistic representation of the results is a powerful analysis technique.

A computer simulation begins with a set of input parameters that define the properties of the system. These parameters are often determined experimentally and carry known uncertainties, and it is important to know how this uncertainty propagates through the simulations. Confidence intervals (estimated ranges of values) are necessary because without some measure of

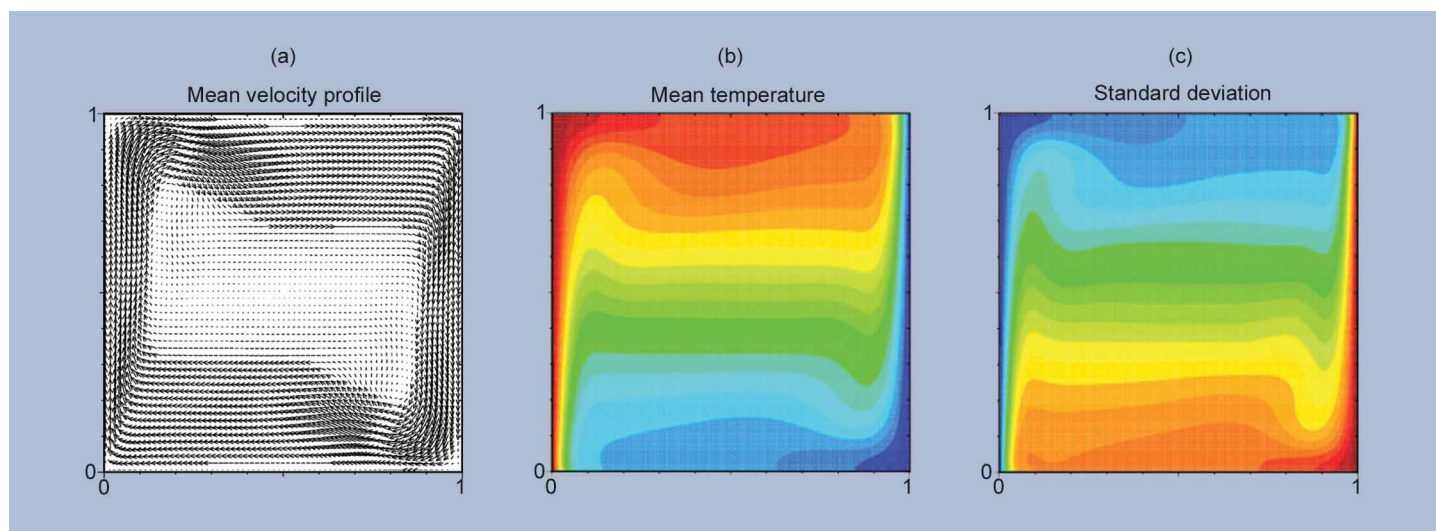
uncertainty in the results, experimental and computational results cannot be compared.

The simplest approach to studying UQ is through straightforward Monte Carlo (MC) simulations. For a more rigorous treatment of UQ, a formalism has been developed using polynomial chaos (PC) expansions. Each uncertain parameter is treated as a stochastic quantity with a known probability density function (PDF). The model solution can also be represented by a PC expansion, which can be used to reconstruct the PDF of the solution.

These concepts can be implemented several ways. The simplest case, known as non-intrusive spectral projection, involves generating many deterministic realizations of the model while sampling parameters from a preselected PDF. A simple projection formalism allows one to compute the coefficients of the PC expansion of the solution from the set of individual realizations. UQ analysis can also be done "intrusively" by reformulating the governing equations to represent each quantity as a PC expansion. The former method is simple to implement but requires a large number of deterministic realizations to converge; the latter method demands the creation of a new code, but total computing time may be several orders of magnitude less.

The Sandia-led group studied two-dimensional natural convection in a heated cavity with an uncertain or stochastic boundary condition. They considered a square cavity filled with a Newtonian fluid, with insulated top and bottom walls, a hot wall to the left and a cold wall to the right. While the hot wall is maintained at a constant temperature, the cold wall may undergo stochastic fluctuations. This creates a distribution of temperature profiles for a specific correlation length and variance. Natural convection within the cavity is modeled as two-dimensional zero-Mach number flow. The goal of the analysis was to understand how the uncertainty in wall temperature affected the predicted properties of the system.

Figure 1a shows the computed mean velocity profile. The arrows indicate the clockwise convection of fluid within the cavity. Figure 1b shows the mean temperature profile, while Figure 1c indicates the standard deviation of the temperature. The net effect of the stochastic nature of the cold wall is evident. The plot of standard deviation shows the accumulation of uncertainty (large standard deviation) along the right side of the cavity.



**Figure 1.** Results computed from uncertainty quantification studies of fluid motion for a Newtonian fluid within a square cavity having insulated top and bottom walls and a hot wall to the left and a cold wall to the right. In panel (a) the magnified arrows show the clockwise convection of the fluid. The net effect of the cold wall is evident in the mean temperature profile of panel (b) which displays the variation of temperatures as false colors with red being the hottest at the top of the cavity and blue being the coolest at the bottom of the cavity. The plot of standard deviation in panel (c) shows the accumulation of uncertainty along the right side of the cavity. The standard deviation decreases from red to blue.





The effect of the temperature fluctuations proceeds down the wall and across the cavity to the hot wall, where diffusion of heat into the fluid reduces the temperature uncertainty. Therefore, the fluid at the top of the cavity has minimal variance.

By representing the response of the system as a PC expansion, you not only get bulk statistics, but you can also determine how each stochastic mode of the boundary condition propagates through the model. The first temperature mode, a roughly uniform distribution, contributes uncertainty in a form similar to that described above.

Mode 2, representing a wall profile with hotter and colder regions, has both positive and negative contributions to the mean temperature distribution that propagate across the cavity. The higher frequency modes have more localized effects and are approximately an order of magnitude smaller. The total standard deviation is a weighted sum of all stochastic modes, so this formulation allows us to determine to what extent each mode contributes most toward the total uncertainty.

Current applications of UQ include evaluating uncertainty propagation in

complex chemical mechanisms, one-dimensional reacting-flow problems, and microchannel flow. Any model parameter—reaction rate pre-exponentials, heats of formation, transport properties—may be represented stochastically and propagated into the simulated system. This assesses not only whether a model produces a “correct” answer, but also determines the ability of a given model to produce meaningful results given the inherent uncertainty in the properties that characterize the physical system—a measure of robustness.

## New Website for Thermochemistry Data

A new site designed to provide thermochemistry data for high-temperature gas-phase and condensed-phase species is now available. Gas-phase data are obtained from quantum-chemistry calculations; condensed-phase data are derived from the modeling phase-diagrams and experimental activity data. The data available currently includes heats of formation, enthalpies, entropies, and heat capacities. Check out the website at <http://www.ca.sandia.gov/HiTempThermo> and look for a more complete description of the website in the next issue of the CRF News (Nov/Dec).

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